

Mathematical Issues for Multiscale Science

- Many tools
 - Need extension
 - Need development
- New ideas
- “No low hanging fruit; many choice nuggets”

Asymptotic and multiscale analysis

- Renormalization group (difficult to apply)
- Homogenization (assumes scale separation)
- Hybrid numerics
- Averaged equations (also called modeling)
- Reduced systems (also an aspect of modeling)
- Parameter passing (assumes scale separation)
- Asymptotic expansions
- AMR

Averaged equations, etc.

- Too many theories (but not the right ones?)
 - Too few validations
 - Too few facts
 - Validation depends on overlapping simulation domains for microphysical and macro simulations
 - Also on experimental data and data analysis
- UQ: provide error bars
 - Error bars for experimental data
 - For simulation
 - For the models
 - Application specific for tight coupling
- AUQ for AMP (automatic uncertainty quantification for automatic multiscale physics)

Hybrid numerics, etc.

- How to couple between different models, different physical descriptions, and different scales
- Requires a (generally new level of) understanding of the relation between the physics and the scales
 - Homogenization
 - Riemann solvers (for fronts)
 - Asymptotics

Validation across lengths scales

- Typical case: subscales are chaotic, macro scales regular
 - Find stable variables of macro system
 - Simulate fine scale and analyze stable features
 - In the case of averaged equations, this is a statistical analysis of moments (averages). Thus the micro simulation is used to produce averaged results, and these are compared with a direct solution of the averaged equations
 - Experimental validation: ideally for both the micro and macro scale simulations

Validation: Is the model (etc.) right?

- Numerical validation proceeds by comparison of more to less exact model, of one model to another, or of model to “exact”
- Experimental validation
- Multiscale data analysis